

**System, Method and Computer Program Product For Fast  
and Efficient Searching of Large Chemical Libraries**

*Abstract*

A system, method, and computer program product for fast and efficient searching of large virtual combinatorial libraries based on a fitness function.

According to the method of the present invention, a first set of N reagent combinations are selected, for example, at random, from a virtual combinatorial library. Each reagent combination in the first set is then enumerated to produce a first set of enumerated compounds. M number of compounds of the first set of enumerated compounds are selected based on the fitness function. The M compounds are then deconvoluted into reagents to generate a focused library. Substantially every reagent combination associated with the focused library is enumerated to produce a second set of enumerated compounds. K number of compounds of the second set of enumerated compounds are then selected based on the fitness function. These K compounds represent a near optimal selection of compounds based on the fitness function.